

# Kernel Methods

## - Generalization -

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based on L. Ralaivola's course on statistical learning theory

# Outline

Rademacher Generalization Bounds

## Focus: generalization bounds

### Targetted result

$\mathcal{H}$  a family of function.  $\forall \delta \in (0, 1]$ , with probability at least  $1 - \delta$  over the random draw of  $S = \{(X_i, Y_i)\}_{i=1}^n$  the following holds

$$\forall h \in \mathcal{H}, \quad \mathbb{E}_{XY} \ell(h, X, Y) \leq \frac{1}{n} \sum_{i=1}^n \ell(h, X_i, Y_i) + \varepsilon \left( \frac{1}{\delta}, \frac{1}{n}, \dots \right).$$

For binary classification we may want something like: with prob.  $1 - \delta$

$$\forall h \in \mathcal{H}, \mathbb{P}_{XY}(h(X) \neq Y) \leq \hat{R}(h, S) + \varepsilon \left( \frac{1}{\delta}, \frac{1}{n}, \dots \right).$$

### Remark (On $\varepsilon$ )

- ▶ decreases when  $n$  increases and when  $\delta$  increases
- ▶ usually contains something related to the *capacity* of  $\mathcal{H}$

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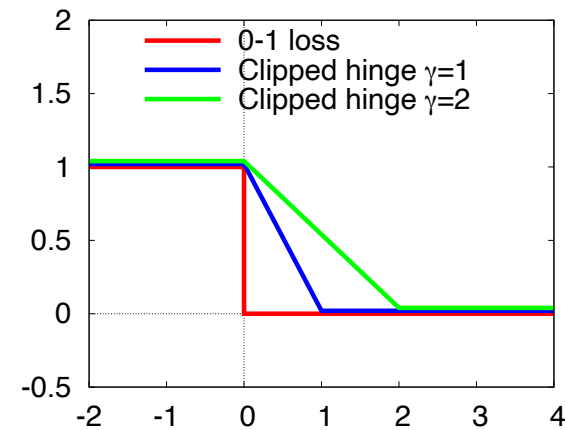
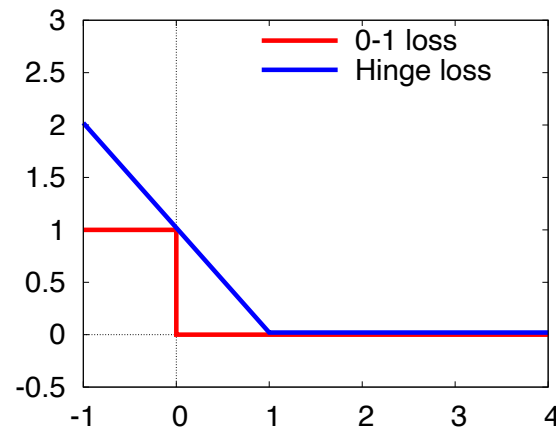
### Remark

Many ways to get generalization bounds

- ▶ VC dimension-based arguments [Vapnik, 1998]
- ▶ PAC-Bayesian theory [McAllester, 1999]
- ▶ Algorithmic stability theory [Bousquet and Elisseeff, 2002]
- ▶ Rademacher-complexity based arguments (our focus) [Bartlett and Mendelson, 2002]
- ▶ ...

# Generalization bounds for binary kernel classifiers (e.g. SVMs)

## 0-1 loss and upper bounds

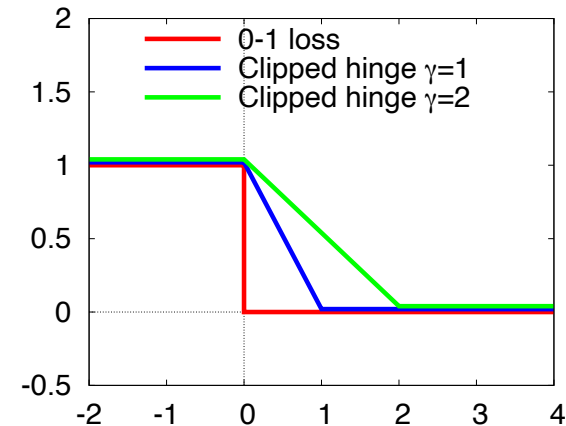
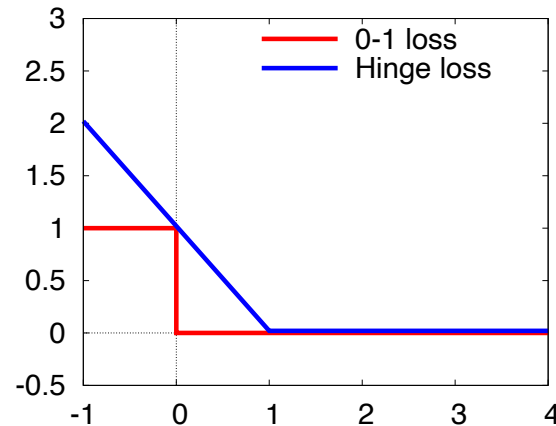


## Clipped loss $\ell_\gamma^c$

$$\ell_\gamma^c(\theta) = \begin{cases} 1 & \text{if } \theta \leq 0 \\ 1 - \theta/\gamma & \text{if } 0 < \theta \leq \gamma \\ 0 & \text{otherwise.} \end{cases}$$

# Generalization bounds for binary kernel classifiers (e.g. SVMs)

## 0-1 loss and upper bounds



## Remark (On the clipped hinge loss)

- ▶ Upper bound on the 0-1 binary loss:  $\forall \theta, 0 \leq \ell_{0-1}(\theta) \leq \ell_{\gamma}^c(\theta)$
- ▶ The empirical clipped  $\hat{R}_{\ell_{\gamma}^c}(h, S)$  risk is  $\hat{R}_{\ell_{\gamma}^c}(h, S) = \frac{1}{n} \sum_{i=1}^n \ell_{\gamma}^c(Y_i h(X_i))$
- ▶ It is  $1/\gamma$ -Lipschitz:

$$\forall \theta, \theta', |\ell_{\gamma}^c(\theta) - \ell_{\gamma}^c(\theta')| \leq \frac{1}{\gamma} |\theta - \theta'|$$

# Generalization bounds for binary kernel classifiers (e.g. SVMs)

## Assumptions

- ▶  $k$ , a bounded Mercer kernel:  $\sup k(X, X) \leq R^2$
- ▶ Bounded norm functions

$$\mathcal{H}_\Lambda = \left\{ \mathbf{x} \mapsto \sum_i \alpha_i k(\mathbf{x}_i, \mathbf{x}), \{ \mathbf{x}_1, \dots, \mathbf{x}_n \} \in \mathcal{X}^n, \|f\|^2 = \sum_{ij} \alpha_i \alpha_j k(\mathbf{x}_i, \mathbf{x}_j) \leq \Lambda^2 \right\}$$

Theorem (Rademacher generalization bound for kernel classifiers  
[Bartlett and Mendelson, 2002, Shawe-Taylor and Cristianini, 2004])

$\forall \delta \in [0, 1)$ , with probability at least  $1 - \delta$ ,  $\forall h \in \mathcal{H}_\Lambda$ ,

$$\mathbb{P}_{XY}(Yh(X) \leq 0) \leq \underbrace{\frac{1}{n} \sum_{i=1}^n \ell_\gamma^c(Y_i h(X_i))}_{\hat{R}_{\ell_\gamma^c}(h, S)} + \frac{c_1 \Lambda}{\gamma n} \sqrt{\sum_{i=1}^n k(X_i, X_i)} + c_2 \sqrt{\frac{\ln 4/\delta}{2n}}$$

where  $c_1, c_2 > 0$ .



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## Remark

- ▶ *Data-dependent* generalization bound
- ▶ Since  $\sqrt{\sum_{i=1}^n k(X_i, X_i)} \leq \Lambda\sqrt{n}$ , at least a  $O(1/\sqrt{n})$  decreasing rate

## Diving into the proof (coooooooooo !!)

Theorem ([McDiarmid, 1989])

Let  $X_1, \dots, X_n$  be independent random variables taking values in a set  $\mathcal{X}$ .

Assume that  $f : \mathcal{X}^n \rightarrow \mathbb{R}$  satisfies

$$\sup_{\mathbf{x}_1, \dots, \mathbf{x}_n, \mathbf{x}'_i \in \mathcal{X}} |f(\mathbf{x}_1, \dots, \mathbf{x}_n) - f(\mathbf{x}_1, \dots, \mathbf{x}_{i-1}, \mathbf{x}'_i, \mathbf{x}_{i+1}, \dots, \mathbf{x}_n)| \leq c_i$$

for every  $1 \leq i \leq n$ . Then, for every  $t > 0$ ,

$$P \{ |f(X_1, \dots, X_n) - \mathbb{E}f(X_1, \dots, X_n)| \geq t \} \leq 2 \exp \left( - \frac{2t^2}{\sum_{i=1}^n c_i^2} \right).$$

Remark

A generalization of Chernoff-Hoeffding bounds. Indeed, if

$f(\mathbf{x}_1, \dots, \mathbf{x}_n) = \frac{1}{n} \sum_{i=1}^n x_i$  and  $X_i \in [a, b]$  and IID, then

$$\sup_{\mathbf{x}_1, \dots, \mathbf{x}_n, \mathbf{x}'_i \in \mathcal{X}} |f(\mathbf{x}_1, \dots, \mathbf{x}_n) - f(\mathbf{x}_1, \dots, \mathbf{x}_{i-1}, \mathbf{x}'_i, \mathbf{x}_{i+1}, \dots, \mathbf{x}_n)| \leq \frac{|b-a|}{n}$$

and

$$P \left\{ \left| \frac{1}{n} \sum_{i=1}^n X_i - \mathbb{E}X \right| \geq t \right\} \leq 2 \exp \left( - \frac{2nt^2}{(b-a)^2} \right).$$

Diving into the proof (cooooooooool !!)

$$\mathbb{P}_{XY}(Yh(X) \leq 0) = \mathbb{E}_{XY} \ell_{0-1}(Yh(X))$$

Diving into the proof (cooooooooool !!)

$$\begin{aligned}\mathbb{P}_{XY}(Yh(X) \leq 0) &= \mathbb{E}_{XY} \ell_{0-1}(Yh(X)) \\ &\leq \mathbb{E}_{XY} \ell_{\gamma}^c(Yh(X))\end{aligned}$$

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## Diving into the proof (oooooooooooool !!!)

Let us take care of  $\sup_{h \in \mathcal{H}_\Lambda} [\mathbb{E}_{X,Y} \ell_\gamma^c(Yh(X)) - \frac{1}{n} \sum_{i=1}^n \ell_\gamma^c(Y_i h(X_i))]$ :

The function

$$H((\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)) := \sup_{h \in \mathcal{H}_\Lambda} \left[ \mathbb{E}_{X,Y} \ell_\gamma^c(Yh(X)) - \frac{1}{n} \sum_{i=1}^n \ell_\gamma^c(y_i h(\mathbf{x}_i)) \right]$$

is such that

$$\sup_{(\mathbf{x}_i, y_i), (\mathbf{x}'_i, y'_i)} \left| H((\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)) - H((\mathbf{x}_1, y_1), \dots, (\mathbf{x}'_i, y'_i), \dots, (\mathbf{x}_n, y_n)) \right| \leq \frac{1}{n}$$

Hence, using McDiarmid's inequality

$$\mathbb{P}_S \left( |\mathbb{E}_{S'} H(S') - H(S)| \geq t \right) \leq 2 \exp \left( -2nt^2 \right)$$

Or, solving for  $2 \exp \left( -2nt^2 \right) = \delta$ , with prob. at least  $1 - \delta$

$$H(S) \leq \mathbb{E}_{S'} H(S') + \sqrt{\frac{\log 2/\delta}{2n}}$$



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The function

$$H((\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)) := \sup_{h \in \mathcal{H}_\Lambda} \left[ \mathbb{E}_{XY} \ell_\gamma^c(Yh(X)) - \frac{1}{n} \sum_{i=1}^n \ell_\gamma^c(y_i h(\mathbf{x}_i)) \right]$$

is such that

$$\sup_{(\mathbf{x}_i, y_i), (\mathbf{x}'_i, y'_i)} \left| H((\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)) - H((\mathbf{x}_1, y_1), \dots, (\mathbf{x}'_i, y'_i), \dots, (\mathbf{x}_n, y_n)) \right| \leq \frac{1}{n}$$

Hence, using McDiarmid's inequality

$$\mathbb{P}_S \left( |\mathbb{E}_{S'} H(S') - H(S)| \geq t \right) \leq 2 \exp \left( -2nt^2 \right)$$

In other words, with probability at least  $1 - \delta$

$$\begin{aligned} & \sup_{h \in \mathcal{H}_\Lambda} \left[ \mathbb{E}_{XY} \ell_\gamma^c(Yh(X)) - \frac{1}{n} \sum_{i=1}^n \ell_\gamma^c(Y_i h(X_i)) \right] \\ & \leq \mathbb{E}_S \sup_{h \in \mathcal{H}_\Lambda} \left[ \mathbb{E}_{XY} \ell_\gamma^c(Yh(X)) - \hat{R}_{\ell_\gamma^c}(h, S) \right] + \sqrt{\frac{\log 2/\delta}{2n}} \end{aligned}$$

## Diving into the proof (cooooooooooooool !!!)

Going back where we left off, with probability at least  $1 - \delta$

$$\mathbb{P}_{XY}(Yh(X) \leq 0) \leq \hat{R}_{\ell_{\gamma}^c}(h, S) + \mathbb{E}_S \sup_{h \in \mathcal{H}_{\Lambda}} \left[ \mathbb{E}_{XY} \ell_{\gamma}^c(Yh(X)) - \hat{R}_{\ell_{\gamma}^c}(h, S) \right] + \sqrt{\frac{\log 2/\delta}{2n}}$$

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Now, let us deal with the second term of the right-hand side:

$$\begin{aligned} \mathbb{E}_S \sup_{h \in \mathcal{H}_\Lambda} \left[ \mathbb{E}_{XY} \ell_\gamma^c(Yh(X)) - \hat{R}_{\ell_\gamma^c}(h, S) \right] \\ = \mathbb{E}_S \sup_{h \in \mathcal{H}_\Lambda} \left[ \mathbb{E}_{S'} \hat{R}_{\ell_\gamma^c}(h, S') - \hat{R}_{\ell_\gamma^c}(h, S) \right] \end{aligned}$$

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because sup is convex (this is *Jensen's inequality* applied to this function)

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$$= \mathbb{E}_{SS'} \sup_{h \in \mathcal{H}_\Lambda} \left[ \frac{1}{n} \sum_{i=1}^n \left( \ell_\gamma^c(Y'_i h(X'_i)) - \ell_\gamma^c(Y_i h(X_i)) \right) \right]$$

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Take a deep breath, and let us keep dealing with this second term

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where  $\mathbb{P}(\sigma_i = +1) = \mathbb{P}(\sigma_i = -1) = 1/2$  and we used that  $S$  and  $S'$  are IID



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$$\leq \mathbb{E}_{SS' \underline{\sigma} \underline{\sigma}'} \sup_{h \in \mathcal{H}_\Lambda} \left[ \frac{1}{n} \sum_{i=1}^n \sigma'_i \ell_\gamma^c(Y'_i h(X'_i)) - \frac{1}{n} \sum_{i=1}^n \sigma_i \ell_\gamma^c(Y_i h(X_i)) \right]$$

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$$\begin{aligned} \mathbb{E}_S \sup_{h \in \mathcal{H}_\Lambda} \left[ \mathbb{E}_{XY} \ell_\gamma^c(Yh(X)) - \hat{R}_{\ell_\gamma^c}(h, S) \right] \\ &= \mathbb{E}_{SS'} \sup_{h \in \mathcal{H}_\Lambda} \left[ \frac{1}{n} \sum_{i=1}^n (\ell_\gamma^c(Y'_i h(X'_i)) - \ell_\gamma^c(Y_i h(X_i))) \right] \\ &= \mathbb{E}_{SS' \underline{\sigma}} \sup_{h \in \mathcal{H}_\Lambda} \left[ \frac{1}{n} \sum_{i=1}^n \sigma_i (\ell_\gamma^c(Y'_i h(X'_i)) - \ell_\gamma^c(Y_i h(X_i))) \right] \end{aligned}$$

where  $\mathbb{P}(\sigma_i = +1) = \mathbb{P}(\sigma_i = -1) = 1/2$  and we used that  $S$  and  $S'$  are IID

$$\begin{aligned} &\leq \mathbb{E}_{SS' \underline{\sigma} \underline{\sigma}'} \sup_{h \in \mathcal{H}_\Lambda} \left[ \frac{1}{n} \sum_{i=1}^n \sigma'_i \ell_\gamma^c(Y'_i h(X'_i)) - \frac{1}{n} \sum_{i=1}^n \sigma_i \ell_\gamma^c(Y_i h(X_i)) \right] \\ &\leq \mathbb{E}_{S \underline{\sigma}} \frac{2}{n} \sup_{h \in \mathcal{H}_\Lambda} \left| \sum_{i=1}^n \sigma_i \ell_\gamma^c(Y_i h(X_i)) \right| \end{aligned}$$

## Diving into the proof (oooooooooooool !!!)

Going back where we left off, with probability at least  $1 - \delta$

$$\mathbb{P}_{XY}(Yh(X) \leq 0) \leq \hat{R}_{\ell_\gamma^c}(h, S) + \mathbb{E}_S \sup_{h \in \mathcal{H}_\Lambda} \left[ \mathbb{E}_{XY} \ell_\gamma^c(Yh(X)) - \hat{R}_{\ell_\gamma^c}(h, S) \right] + \sqrt{\frac{\log 2/\delta}{2n}}$$

This second term is resilient, but we are almost there

$$\mathbb{E}_S \sup_{h \in \mathcal{H}_\Lambda} \left[ \mathbb{E}_{XY} \ell_\gamma^c(Yh(X)) - \hat{R}_{\ell_\gamma^c}(h, S) \right] \leq \mathbb{E}_{S \underline{\sigma}} \frac{2}{n} \sup_{h \in \mathcal{H}_\Lambda} \left| \sum_{i=1}^n \sigma_i \ell_\gamma^c(Y_i h(X_i)) \right|$$

## Diving into the proof (cooooooooooooool !!!)

Going back where we left off, with probability at least  $1 - \delta$

$$\mathbb{P}_{XY}(Yh(X) \leq 0) \leq \hat{R}_{\ell_\gamma^c}(h, S) + \mathbb{E}_S \sup_{h \in \mathcal{H}_\Lambda} \left[ \mathbb{E}_{XY} \ell_\gamma^c(Yh(X)) - \hat{R}_{\ell_\gamma^c}(h, S) \right] + \sqrt{\frac{\log 2/\delta}{2n}}$$

This second term is resilient, but we are almost there

$$\begin{aligned} \mathbb{E}_S \sup_{h \in \mathcal{H}_\Lambda} \left[ \mathbb{E}_{XY} \ell_\gamma^c(Yh(X)) - \hat{R}_{\ell_\gamma^c}(h, S) \right] &\leq \mathbb{E}_{S \underline{\sigma}} \frac{2}{n} \sup_{h \in \mathcal{H}_\Lambda} \left| \sum_{i=1}^n \sigma_i \ell_\gamma^c(Y_i h(X_i)) \right| \\ &\leq \underbrace{\frac{2}{\gamma} \mathbb{E}_{S \underline{\sigma}} \sup_{h \in \mathcal{H}_\Lambda} \frac{2}{n} \left| \sum_{i=1}^n \sigma_i h(X_i) \right|}_{\text{see [Bartlett and Mendelson, 2002]}} \end{aligned}$$

## Rademacher complexity of $\mathcal{H}_\Lambda$

### Definition

$$\mathcal{R}(\mathcal{H}_\Lambda) = \mathbb{E}_{S, \underline{\sigma}} \sup_{h \in \mathcal{H}_\Lambda} \frac{2}{n} \left| \sum_{i=1}^n \sigma_i h(X_i) \right|$$

is the *Rademacher complexity* of  $\mathcal{H}_\Lambda$

### Remark

- ▶ It measures the richness of the class  $\mathcal{H}_\Lambda$
- ▶ Based on how well the class of functions is capable of correlating with randomly assigned labels
- ▶ The marginal distribution over  $\mathcal{X}$  is directly taken into account

### Definition (Empirical Rademacher complexity $\hat{\mathcal{R}}(\mathcal{H}_\Lambda, S)$ )

The *empirical Rademacher Complexity* of  $\mathcal{H}_\Lambda$  is defined as

$$\hat{\mathcal{R}}(\mathcal{H}_\Lambda, S) := \mathbb{E}_{\underline{\sigma}} \sup_{h \in \mathcal{H}_\Lambda} \frac{2}{n} \left| \sum_{i=1}^n \sigma_i h(X_i) \right|$$

## Rademacher complexity of $\mathcal{H}_\Lambda$

### Concentration of $\hat{\mathcal{R}}(\mathcal{H}_\Lambda, S)$

$\hat{\mathcal{R}}(\mathcal{H}_\Lambda, S)$  is a concentrated variable. Using McDiarmid inequality again, we obtain that, with probability at least  $1 - \delta$

$$\mathcal{R}(\mathcal{H}_\Lambda) \leq \hat{\mathcal{R}}(\mathcal{H}_\Lambda, S) + c \sqrt{\frac{\log 2/\delta}{2n}}$$

### Bounding $\hat{\mathcal{R}}(\mathcal{H}_\Lambda, S)$

$$\begin{aligned} \hat{\mathcal{R}}(\mathcal{H}_\Lambda, S) &= \mathbb{E}_{\underline{\sigma}} \sup_{h \in \mathcal{H}_\Lambda} \frac{2}{n} \left| \sum_{i=1}^n \sigma_i h(X_i) \right| = \mathbb{E}_{\underline{\sigma}} \sup_{h \in \mathcal{H}_\Lambda} \frac{2}{n} \left| \sum_{i=1}^n \sigma_i \langle h, k(X_i, \cdot) \rangle \right| \\ &= \mathbb{E}_{\underline{\sigma}} \sup_{h \in \mathcal{H}_\Lambda} \frac{2}{n} \left| \left\langle h, \sum_{i=1}^n \sigma_i k(X_i, \cdot) \right\rangle \right| \\ &= \mathbb{E}_{\underline{\sigma}} \frac{2}{n} \Lambda \left\| \sum_{i=1}^n \sigma_i k(X_i, \cdot) \right\| = \mathbb{E}_{\underline{\sigma}} \frac{2}{n} \Lambda \sqrt{\sum_{ij} \sigma_i \sigma_j k(X_i, X_j)} \\ &\leq \frac{2}{n} \Lambda \sqrt{\mathbb{E}_{\underline{\sigma}} \sum_{ij} \sigma_i \sigma_j k(X_i, X_j)} = \frac{2}{n} \Lambda \sqrt{\sum_i k(X_i, X_i)} \end{aligned}$$

## Closing the proof

We had

$$\mathbb{P}_{XY}(Yh(X) \leq 0) \leq \hat{R}_{\ell_\gamma^c}(h, S) + \mathbb{E}_S \sup_{h \in \mathcal{H}_\Lambda} \left[ \mathbb{E}_{XY} \ell_\gamma^c(Yh(X)) - \hat{R}_{\ell_\gamma^c}(h, S) \right] + \sqrt{\frac{\log 2/\delta}{2n}}$$

and

$$\mathbb{E}_S \sup_{h \in \mathcal{H}_\Lambda} \left[ \mathbb{E}_{XY} \ell_\gamma^c(Yh(X)) - \hat{R}_{\ell_\gamma^c}(h, S) \right] \leq \frac{2}{\gamma} \mathbb{E}_{S\sigma} \sup_{h \in \mathcal{H}_\Lambda} \frac{2}{n} \left| \sum_{i=1}^n \sigma_i h(X_i) \right|$$

and we just proved

$$\mathbb{E}_{S\sigma} \sup_{h \in \mathcal{H}_\Lambda} \frac{2}{n} \left| \sum_{i=1}^n \sigma_i h(X_i) \right| \leq \frac{2}{n} \Lambda \sqrt{\sum_i k(X_i, X_i)} + c \sqrt{\frac{\log 2/\delta}{2n}}$$

Combining everything and adjusting some constants give the desired result

$$\mathbb{P}_{XY}(Yh(X) \leq 0) \leq \hat{R}_{\ell_\gamma^c}(h, S) + \frac{c_1 \Lambda}{\gamma n} \sqrt{\sum_{i=1}^n k(X_i, X_i)} + c_2 \sqrt{\frac{\ln 4/\delta}{2n}}$$

## Partial conclusion

### Generalization bounds

- ▶ are easy to derive for kernel classifiers
- ▶ can still be improved
- ▶ need for practical bounds (such as leave-one-out bounds)
- ▶ ...



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